The Protofilaments number effect in the mechanical characterization of the β_2 microglobulin amyloid fibrils

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Recent experimental studies show the existence of the various protofilaments number of amyloid fibrils which are related to the structural and mechanical characteristics. Moreover, the number of protofilaments can affect to the toxicity of the amyloid fibrils in the early aggregation states, and infectivity in the growth mechanism of prion protein in the prion states. Here, we investigate the structural and mechanical characteristics of the β_2 microglobulin amyloid fibrils with respect to the number of protofilaments with using molecular dynamic simulation and elastic network model. The molecular structures of four kinds of protofilaments are successfully constructed, the pitch increases linearly with the protofilaments number comparable to the experimental result. The mechanical properties of the β_2 microglobulin amyloid fibrils linearly increase with the protofilaments number, which are well explained by the varied Timoshenko beam theory. Finally, the sequence mutation and polymorphs effects in the mechanical characteristics are studied which are comparable to the experimental result and simulational results for the other amyloid fibrils. Our results also indicate structure-property relationship in the amyloid fibrils which can shed light on the elucidating the aggregation states in the amyloid-related diseases.

Keywords: amyloid, β_2 microglobulin, protofilament number, mechanical property, elastic network model, normal mode analysis

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